TT 19: CE: Metal-Insulator Transition 2

Time: Wednesday 9:30–13:00 Location: H18

TT 19.1 Wed 9:30 H18

Charge, orbital and magnetic ordering in $La_{0.4}Sr_{1.6}MnO_4$ — •Holger Ulbrich[1], Daniel Senff[1], Olaf J. Schumann[1], Yvan Sidis[2], Paul Steffens[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin, Saclay — [3]Institut Laue Langevin, Grenoble

The coupled ordering of charge orbital and spin (COS) degrees of freedom in the manganites constitutes a key element to understand the mechanism of CMR. 214 manganites are well-suited to study the COS state. The COS state of the half-doped layered material $La_{0.5}Sr_{1.5}MnO_4$ can be described by the Goodenough model [1-3]. The over-doped $La_{0.4}Sr_{1.6}MnO_4$ consists of 60% Mn^{4+} ions and 40% Mn^{3+} ions. Consequently there is no optimal checkerboard charge ordering possible. We suggest to put these excess of Mn^{4+} ions into stripes cutting the zig-zag chains. Investigations by neutron scattering emphasize this idea as incommensurable superstructure reflections of charges and orbitals could be found. The reflections of the magnetic ordering of Mn^{3+} are incommensurable as well, while the magnetic ordering of Mn^{4+} yields scattering at commensurable positions. These experiments are not in agreement with results by Larochelle *et al.* [4]. Stripe-like arrangement of Mn^{4+} ions are similar to the stripe phases in nickelates and cuprates. The order, however, is quite complex involving incommensurate ordering of orbitals, charges and Mn^{3+}-magnetic moments.

[1] D. Senff, *et al.*, Phys. Rev. Lett. 96, 257201 (2006).
[2] D. Senff, et al., Phys. Rev. B 77, 184413 (2008).
[3] J.B. Goodenough, Phys. Rev. 100, 564 (1955).
[4] S. Larochelle *et al.*, Phys. Rev. B 71, 024435 (2005).

TT 19.2 Wed 9:45 H18

Comparison of EELS and RIXS measurements for the single layer manganite $La_{1-x}Sr_{1+x}MnO_4$ — •Roberto Kraus[1], Jochen Geck[1], Matthias Schrade[1], Martin Knupfer[1], Bernd Büchner[1], and Pieter Glatzel[2] — [1]IFW Dresden, Germany — [2]ESRF Grenoble, France

The manganites show a variety of magnetic and electronic phases which are connected to charge, spin and orbital degrees of freedom. One example is the single layered perovskite $La_{1-x}Sr_{1+x}MnO_4$. Upon hole doping new in-gap excitations appear and up to now it is unclear if they are of charge-transfer or Mott-Hubbard type. To characterize the excitations in the system, we performed electron energy-loss spectroscopy (EELS) and resonant inelastic X-ray scattering (RIXS) of the Mn K-edge. The observed in-gap excitation shows a small positive dispersion and a clear positive shift as a function of temperature in the half-doped sample.

TT 19.3 Wed 10:00 H18

Orbital order in $La_{0.5}Sr_{1.5}MnO_4$: a failure of the local Jahn-Teller physics — •Hua Wu[1], C. F. Chang[1], Z. Hu[1], O. Schumann[1], J. C. Cezar[2], T. Burnus[1], N. Hollmann[1], N. B. Brookes[2], A. Tanaka[3], M. Braden[1], D. I. Khomskii[1], and L. H. Tjeng[4] — [1]II. Phys. Inst, Uni Köln — [2]ESRF, Grenoble, France — [3]Hiroshima Univ. Japan — [4]MPI Dresden

Orbital order (OO) occurs quite often in orbitally degenerate correlated transition-metal compounds. It has been generally accepted that there is one-to-one correspondence between a specific orbital order and a local Jahn-Teller distortion. Here we demonstrate that this is not always true, by demonstrating a failure of the local Jahn-Teller physics in the single-layered perovskite $La_{0.5}Sr_{1.5}MnO_4$ which is one of prototype OO materials. We studied both the site- and bond-centered charge orderings, crystal field levels, orbital states and their dependence on the varying local lattice distortions, through detailed ab initio electronic structure calculations. We conclude that this material has the site-centered charge ordering, and that the local Jahn-Teller physics fails and the type of occupied orbitals ($3x^2{-}r^2/3y^2{-}r^2$ ones) contradicts the local compression of $Mn^{3+}O_6$ octahedra which could require $x^2{-}z^2/y^2{-}z^2$ occupation. We explain this by the contribution of the long-range crystal-field in this anisotropic layered material and by the maximization of kinetic energy. Our theoretical results are confirmed by x-ray absorption linear dichroism.

TT 19.4 Wed 10:15 H18

Structural transformations due to electronic correlations in paramagnetic $KCuF_3$ and $LaMnO_3$ — •Ivan Leonov[1], Dmitry Korotin[2], Nadia Binggeli[3], Vladimir I. Anisimov[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Institute of Metal Physics, Yekaterinburg, Russia — [3]ICTP and INFM-CNR Democritos National Simulation Center, Trieste, Italy

We present a computational scheme for *ab initio* total-energy calculations of materials with strongly interacting electrons using a plane-wave basis set [1]. It combines *ab initio* band structure and dynamical mean-field theory and is implemented in terms of plane-wave pseudopotentials. The present approach allows us to investigate complex materials with strongly interacting electrons and is able to treat atomic displacements, and hence structural transformations, caused by electronic correlations. Results obtained for paramagnetic $KCuF_3$ and $LaMnO_3$, namely an equilibrium Jahn-Teller distortion and antiferro-orbital order agree well with experiment. The structural optimization performed for paramagnetic $KCuF_3$ yields the correct lattice constant, equilibrium Jahn-Teller distortion and tetragonal compression of the unit cell. The present approach is able to determine correlation-induced structural transformations, equilibrium atomic positions and lattice structure in both strongly and weakly correlated solids in their *paramagnetic* phases as well as in phases with long-range magnetic order.

[1] I. Leonov, N. Binggeli, Dm. Korotin, V. I. Anisimov, N. Stojić, and D. Vollhardt, Phys. Rev. Lett. **101**, 096405 (2008).

TT 19.5 Wed 10:30 H18

Origin of Jahn-Teller distortion and orbital-order in $LaMnO_3$ — •Eva Pavarini[1] and Erik Koch[2] — [1]IFF und IAS, Forschungszentrum Jülich — [2]GRS, Jülich

The origin of the cooperative Jahn-Teller distortion and orbital-order in $LaMnO_3$ is central to the physics of the manganites. The question is complicated by the simultaneous presence of tetragonal and $GdFeO_3$-type distortions and the strong Hund's rule coupling between e_g and t_{2g} electrons. To clarify the situation we calculate the transition temperature for the Kugel-Khomskii superexchange mechanism by using the local density approximation+dynamical mean-field method, and disentangle the effects of super-exchange from those of lattice distortions. We find that super-exchange alone would yield $T_{KK} \sim 650$ K. The tetragonal and $GdFeO_3$-type distortions, however, reduce T_{KK} to ~ 550 K. Thus electron-phonon coupling is essential to explain the persistence of local Jahn-Teller distortions to $\gtrsim 1150$ K and to reproduce the occupied orbital deduced from neutron scattering.

TT 19.6 Wed 10:45 H18

First principles study of the electronic structure and phonon properties on double-layer manganites — •Omar De la Peña-Seaman, Rolf Heid, and Klaus-Peter Bohnen — Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, Germany

We have studied the electronic and lattice dynamical properties of the tetragonal double-layer manganite system $La_{2-2x}Sr_{1+2x}Mn_2O_7$ ($x = 0.4$) within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation for modeling the alloy. The system has been investigated for non-magnetic and ferromagnetic phases. The performance of LDA and GGA exchange-correlation functionals on the properties under study was analyzed. We have used the experimental lattice constants, optimizing the internal structural parameters for each magnetic phase (non-magnetic and ferromagnetic). The electronic band structure as well as individual contributions to the density of states are discussed. The calculated phonon dispersion in [ξ00] and [ξξ0] high-symmetry directions for different magnetic phases are compared between them and with experimental data available in the literature. In addition, an analysis of the most representative phonon modes is performed, and the electron-phonon couplings discussed in detail.

TT 19.7 Wed 11:00 H18

THz and infrared spectroscopy in $FeCr_2S_4$ — •Joachim Deisenhofer[1], Yurii Goncharov[2], Franz Mayr[1], Dat Quach[3], Joanna Groza[3], Vladimir Tsurkan[1,4], and Alois Loidl[1] — [1]Experimentalphysik V, Center for Electronic Correlations and Mag-

netism, Institute for Physics, Augsburg University, D-86135 Augsburg, Germany — [2]General Physics Institute of the Russian Academy of Sciences, 119991 Moscow, Russia — [3]Department of Chemical Engineering and Materials Science, University of California, Davis, CA 95616, USA — [4]Institute of Applied Physics, Academy of Sciences of Moldova, MD-2028 Chişinău, Republic of Moldova

We investigate the Jahn-Teller transition at T_{JT} = 9K in the CMR system $FeCr_2S_4$ by THz and IR spectroscopy. Below T_{JT} we observe the appearance of new phonon modes in the far-infrared region and new excitations in the THz regime. We attribute the latter to a splitting of the Fe^{2+} ground state due to the transition from a dynamic to a static Jahn-Teller distortion.

Invited Talk TT 19.8 Wed 11:15 H18

Spectroscopy on Strongly Correlated Electron Materials — •Liu Hao Tjeng — Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

One of the most intriguing aspects of transition metal materials is the wide variety of their physical properties. Although conceptually clean and beautiful, theoretical simplifications in terms of, for instance, a single band Hubbard model turn out to be inadequate. It now becomes clear that the interplay between the relevant charge, orbital and spin degrees of freedom of the metal ions involved determines the intricate balance between band formation and electron-correlation effects.

In this talk we would like to illustrate how synchrotron-based electron spectroscopies can contribute to the identification of the key parameters in the electronic structure of transition metal oxides, in particular those showing metal-insulator transitions as a function of temperature or doping. We use a combination of soft-x-ray absorption spectroscopy and photoemission, as well as the newly developed hard-x-ray photoelectron spectroscopy (HAXPES), to address issues related to the inter-site spin-spin and orbital-orbital correlations. Furthermore, we will address how accurate these phenomena can be theoretically described using the LDA+DMFT method and its most recent extensions.

In collaboration with Z. Hu, M. Haverkort, T. Koethe, C.F. Chang, H. Wu, T. Burnus, Y. Chin, N. Hollmann, H. Fujiwara, C. Schußler-Langeheine, H. Roth, M. Benomar, M. Reuther, C. Zobel, T. Lorenz, D. Khomskii, A. Tanaka, E. Pavarini, W. Reichelt, S. Barilo, J. Cezar, N. Brookes, H.H. Hsieh, H.J. Lin, C.T. Chen. Supported by SFB 608.

15 min. break

TT 19.9 Wed 12:00 H18

Absence of an electric potential gradient across the overlayer of $LaAlO_3/SrTiO_3$ heterostructures inferred from XPS — •Götz Berner[1], Michael Sing[1], Stefan Thiel[2], Jochen Mannhart[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Experimentelle Physik VI, Universität Augsburg

The origin of the interface electron gas (2DEG) in $LaAlO_3/SrTiO_3$ oxide heterostructures (LAO/STO) is a heavily discussed topic. Apart from possible influences of oxygen defects recent experimental and theoretical work suggests an electronic reconstruction as the driving mechanism for the 2DEG. In the most simple picture half an electron is transferred from the surface to the interface to neutralize the electric potential piling up across the polar LAO overlayers. Microscopically, density-functional (DFT) calculations find a potential gradient which shifts the LAO electronic states until the valence-band maximum crosses the chemical potential and electrons are transferred from the surface to the STO conduction-band minimum at the interface.

By x-ray photoelectron spectroscopy (XPS) this potential gradient should be observable as a significant broadening of the Al 1*s* core level. Moreover, probing the topmost LAO layer there should appear finite spectral weight at the chemical potential. However, in our XPS studies on several samples with different overlayer thicknesses none of these signatures is observed. In addition, we determined the band offsets of LAO and STO at the interface and arrived at values which suggest a flat band situation in contrast to the DFT calculations.

TT 19.10 Wed 12:15 H18

Possible localization of electrons at $LaAlO_3$-$SrTiO_3$ interfaces at finite temperatures — •Yang-Chung Liao[1], Nicolas Reyren[2], Stefano Gariglio[2], Christoph Richter[1], Rainer Jany[1], Stefan Thiel[1], Martin Breitschaft[1], German Hammerl[1], Thilo Kopp[1], Jean-Marc Triscone[2], and Jochen Mannhart[1] — [1]Experimental Physics VI, Center for Electronic Correlation and Magnetism, University of Augsburg, Augsburg, Germany — [2]DPMC, University of Geneva, Geneva, Switzerland

Intriguingly, the $LaAlO_3$-$SrTiO_3$ ($AlO_2/LaO/TiO_2/SrO$) interface possesses conducting electrons if the $LaAlO_3$ thickness exceeds 3 unit cells. By applying depleting gate fields in field-effect devices at finite temperatures, we observe the conducting interfaces to localize electrons. Below a critical carrier density, the interfaces display nonlinear current-voltage characteristics showing gap-like features. At higher carrier densities, the interface electron system is ohmic with a weak-localization type behavior. Based on current-voltage characteristics and magneto-transport properties, we trace the phase diagram of the $LaAlO_3$-$SrTiO_3$ interface electron system.

TT 19.11 Wed 12:30 H18

Microscopic origin of the electronic reconstruction at the $LaAlO_3/SrTiO_3$ interface — •Andrea Rubano[1], Domenico Paparo[2], Antigone Marino[2], Paolo Perna[2], Umberto Scotti di Uccio[2], Fabio Miletto Granozio[2], Christoph Richter[3], Stefan Paetel[3], Jochen Mannhart[3], Lorenzo Marrucci[2], and Manfred Fiebig[1] — [1]HISKP, Universitaet Bonn, Bonn, Germany — [2]CNR-INFM Coherentia and Dip. di Scienze Fisiche, Università di Napoli Federico II, Italy — [3]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

$LaAlO_3/SrTiO_3$ interfaces are one of the most challenging topics in the field of perovskite oxides. Recently it was observed that a conductive two-dimensional electron gas (2DEG) emerges at the interface of these wide-gap insulators. The 2DEG formation occurs once $n \geq 4$ $LaAlO_3$ monolayers are deposited on top of the $SrTiO_3$. Although some macroscopic models have been proposed, our understanding on the microscopic scale is still at its infancy. Second harmonic (SHG) spectroscopy is an interface-only sensitive technique and, thus, an ideal tool to study these materials. Applying SHG, we demonstrate that a structural reorganization of the interfacial Ti-orbitals already occurs at $n = 3$, yet without any onset of conductivity, because the injected carriers are localized at the interface. The electronic reorganization at $n = 3$ leads to an abrupt increase of the SHG yield due to the enhancement of the polar asymmetry of the Ti 3*d* orbitals, and a crystal field splitting of the $d(xy)$ orbitals is observed.

TT 19.12 Wed 12:45 H18

Electronic reconstruction in thin $LaAlO_3$ films on $SrTiO_3$(001) via a $SrTiO_3$-capping layer — •Katrin Otte[1], Rossitza Pentcheva[1], and Warren E. Pickett[2] — [1]Section Crystallography, Dept. of Earth and Environmental Sciences, University of Munich — [2]Department of Physics, UC Davis

Novel electronic phenomena can be realized at the interface between polar (e.g. $LaAlO_3$) and nonpolar (e.g. $SrTiO_3$) band insulators. An intriguing example is the thickness dependent insulator-to-metal transition in thin $LaAlO_3$ films on $SrTiO_3$(001)[1]. Density functional theory calculations show that a strong lattice polarization allows several layers of $LaAlO_3$ on $SrTiO_3$(001) to remain insulating before an insulator-to-metal transition takes place at around 4 monolayers (MLs)[2]. We demonstrate here that an additional capping $SrTiO_3$ can trigger the electronic reconstruction already at two MLs of $LaAlO_3$. A surface O 2*p* state, similar to the surface states in $SrTiO_3$, is identified as the origin of this additional band shift.

Altogether, the $SrTiO_3$-capping layer represents an alternative pathway to tune the electronic reconstruction of the system leading to the formation of an electron-hole bilayer.

[1] S. Thiel et al., Science **313**, 1942 (2006).
[2] R. Pentcheva and W.E. Pickett, Phys. Rev. Lett. **102**, 107602 (2009).